A NEW METHOD OF AUTOMATIC COMPUTATION OF STELLAR EVOLUTION

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ABSTRACT

A method is described for obtaining time sequences of stellar models describing evolutionary changes. This method is a modified version of an earlier one described by Henyey, Wilets, Böhm, LeLevier, and Levée (1959). The modifications involve the evaluation of all quantities at the same discrete points. The technique provides for coupling the interior integrations to those for model atmospheres based on mixing-length theory. The scope of the formalism is such as to provide for a wide range of calculations for spherically symmetric configurations in hydrostatic equilibrium.

I. INTRODUCTION

A method (Method I) for automatic calculation of stellar evolution using high-speed electronic computers was presented in a previous report (Henyey, Wilets, Böhm, LeLevier, and Levée 1959). The technique developed therein proves to be quite powerful in carrying out the necessary complex computations; nevertheless it contains certain awkward features which require modification. The present paper describes a modified method (Method II) which eliminates the undesirable features of Method I and which is presently in use at Berkeley. Both methods are limited to the investigation of spherically symmetric configurations in hydrostatic equilibrium.

The principal modification involves the manner in which the values of certain physical variables are associated with geometrical position in the configuration. The star is considered to be divided into concentric shells or zones. This reduces the configuration to a one-dimensional system in which the radius is subdivided into zones by a set of mesh points. In Method I the mesh points fall into two classes, such that the points alternate in membership between the classes as one proceeds radially outward. The classes differ in that certain of the variables are evaluated at points in one class and the remaining variables at points in the other. In Method II all quantities are evaluated at the same mesh points. Two advantages result from this revision. One is the more straightforward way in which convective and radiative regions may be joined in Method II. The other advantage is that the errors caused by finite zone sizes are more easily held within reasonable bounds. This is best achieved by using a so-called centered scheme of discretization. In Method I this is done in a rather simple way, which is valid only if the spacing of mesh points is more or less uniform. In the revised method this restriction is removed, and extra mesh points can be inserted locally for finer zoning wherever this is needed to represent rapid spatial variation of physical variables with necessary precision.

II. THE BASIC DIFFERENTIAL EQUATIONS

The development of the modified form of the computational technique requires that the basic equations be put into a suitable form. Let ξ be a Lagrangian variable and let $m(\xi)$ be the mass inclosed within a sphere designated by ξ, that is,

$$m = m(\xi) , \qquad 0 \leq \xi \leq 1 . \tag{1}$$

Here it is understood that

$$m(0) = 0 , \quad \text{and} \quad m(1) = M , \tag{2}$$

where M is the total mass.

The basic equations of stellar structure are written

$$\frac{\partial P}{\partial \xi}+\frac{Gm\rho}{r^2}\frac{\partial r}{\partial \xi}=0\,, \tag{3}$$

$$m'-4\pi r^2\rho\frac{\partial r}{\partial \xi}=0\,, \tag{4}$$

$$\frac{\partial l}{\partial \xi}-m'\left[\epsilon-\frac{\partial E}{\partial t}-P\frac{\partial}{\partial t}\left(\frac{1}{\rho}\right)\right]=0\,; \tag{5}$$

and for radiative-conductive transfer of energy

$$\frac{\partial T}{\partial \xi}+\frac{3\kappa\rho l}{64\pi\sigma T^3 r^2}\frac{\partial r}{\partial \xi}=0\,, \tag{6}$$

(where κ, the opacity, includes the effect of electron conduction) or for convection

$$\frac{\partial E}{\partial \xi}+P\frac{\partial}{\partial \xi}\left(\frac{1}{\rho}\right)=0\,. \tag{7}$$

The symbol m' represents the ordinary derivative of $m(\xi)$ with respect to ξ. As usual ρ represents the density, P the pressure, T the temperature, l the luminosity, and r the radius at any interface within the star. E is the internal energy per unit mass and ϵ the thermonuclear energy release per unit mass and time. M, R, and L are the mass, radius, and luminosity of the whole star.

The discretization of the variables inevitably leads to the use of both differences and averages of neighboring values. The resulting combinations usually represent the desired values most accurately when the operations are carried out on quantities whose variations are as nearly linear as possible. The pressure and density vary in order of magnitude to an extent which precludes their use in differences and averages. To circumvent this difficulty we replace them with the artificial variables

$$p = P^{1/4} \tag{8}$$

and

$$q = \rho^{1/3}\,. \tag{9}$$

The precise exponents, which are somewhat arbitrary, were chosen in analogy with the polytrope of index three. We also find it convenient to moderate the variation of l near the center of the star by the use throughout the star of a pseudoflux, F, defined by

$$l = \xi^2 F\,. \tag{10}$$

Using these three artificial variables and, in addition, making the substitution

$$K=\frac{3\kappa p^3}{256\pi G\sigma T^3}, \tag{11}$$

we obtain the following revised forms of equations (3), (4), and (5):

$$\frac{\partial p}{\partial \xi}+\frac{Gmq^3}{4p^3r^2}\frac{\partial r}{\partial \xi}=0\,, \tag{12}$$

$$m'-4\pi r^2 q^3\frac{\partial r}{\partial \xi}=0\,, \tag{13}$$

$$\xi^2\frac{\partial F}{\partial \xi}+2\xi F-m'\left(\epsilon-\frac{\partial E}{\partial t}+\frac{3p^4}{q^4}\frac{\partial q}{\partial t}\right)=0\,, \tag{14}$$

and combining equation (6) with equation (3)

$$\frac{\partial T}{\partial \xi} - \frac{16K\xi^2 F}{m}\frac{\partial p}{\partial \xi} = 0 \text{ (radiative-conductive transport)}, \tag{15}$$

or

$$\frac{\partial E}{\partial \xi} - \frac{3p^4}{q^4}\frac{\partial q}{\partial \xi} = 0 \text{ (convective transport)}. \tag{16}$$

The outermost regions of a star require a treatment which involves considerable complications and which will be discussed later. Moreover the evolution of a star is largely a result of changes in composition resulting from various nuclear reactions. For the present we shall regard the composition as specified. Brief reference to the problem of time variations in the various nuclear species is made in a later section.

III. THE DIFFERENCE EQUATIONS

The march of the various parameters describing the structure of a configuration must be described by discrete variables. These are evaluated at discrete mass points $\xi_j (j = 0, 1, \ldots, J)$. We assume that these are arranged in order of position, proceeding from the center ($\xi_0 = 0$) to the surface ($\xi_J = 1$). For simplicity we label the different variables with the corresponding subscripts, for example, T_j, q_j, etc.

The choice of the mass points actually used must be based on considerations of accuracy. They must be adequate in number and distribution to insure that the truncation error of the difference equations be held within acceptable bounds. Unfortunately, it is practically impossible to obtain an over-all evaluation of such errors and it is necessary to proceed by using rough criteria based on holding the point-to-point variations within certain limits.

We have found it expedient to recognize two categories of points. One includes a set of points which are never varied in either number or position. The second includes additional points which are interpolated among the fixed ones as needed and may be removed when circumstances permit. Specific criteria for the inclusion and the removal of temporary points are based on the variations of certain representative variables. We have found that the temperature, the fourth root of the pressure, and the abundance of He^4 provide effective and adequate criteria. The decisions concerning these points are made at the completion of the computations for each time step on the basis of the newly derived values.

The following mass variables are needed:

$$m_j = m(\xi_j), \tag{17}$$

$$m_j' = m'(\xi_j), \tag{18}$$

$$m_{j+1/2} = m(\xi_{j+1/2}), \tag{19}$$

and

$$m_{j+1/2}' = m'(\xi_{j+1/2}), \tag{20}$$

where

$$\xi_{j+1/2} = \tfrac{1}{2}(\xi_{j+1} + \xi_j). \tag{21}$$

The procedure to be followed in preparing a difference representation of a differential equation is far from unique. In general, it is desirable to construct a centered form; that is, one which is symmetric in the variables at both points of the interval or zone. In the case of complex equations, considerable choice may still be open. The procedure followed in this method is to average variables whose variation is thought to be most nearly linear.

The system which we adopt, and which is explained subsequently, is as follows. For equation (12):

$$p_{j+1} - p_j + \frac{Gm_{j+1/2}(q_{j+1}+q_j)^3(r_{j+1}-r_j)}{(p_{j+1}+p_j)^3(r_{j+1}+r_j)^2} = 0. \tag{22}$$

For equation (13):

$$\frac{8}{\pi} m_{j+1/2}'(\xi_{j+1}-\xi_j) - (q_{j+1}+q_j)^3(r_{j+1}+r_j)^2(r_{j+1}-r_j) = 0. \tag{23}$$

For equation (14):

$$\begin{aligned} &F_{j+1}(\xi_{j+1}+\xi_j)(3\xi_{j+1}-\xi_j) + F_j(\xi_{j+1}+\xi_j)(\xi_{j+1}-3\xi_j) \\ &- 2m_{j+1/2}'(\xi_{j+1}-\xi_j)\left[2(\epsilon_{j+1}\epsilon_j)^{1/2} - \frac{E_{j+1}+E_j-E_{j+1}^n-E_j^n}{\Delta t}\right. \\ &\left. + 3\left(\frac{p_{j+1}+p_j}{q_{j+1}+q_j}\right)^4 \frac{q_{j+1}+q_j-q_{j+1}^n-q_j^n}{\Delta t}\right] = 0. \end{aligned} \tag{24}$$

For equation (15):

$$T_{j+1} - T_j - \frac{(K_{j+1}+K_j)(\xi_{j+1}+\xi_j)^2(F_{j+1}+F_j)(p_{j+1}-p_j)}{m_{j+1/2}} = 0. \tag{25}$$

For equation (16):

$$E_{j+1} - E_j - 3\left(\frac{p_{j+1}+p_j}{q_{j+1}+q_j}\right)^4 (q_{j+1}-q_j) = 0. \tag{26}$$

The symbols q_j^n and E_j^n represent values of these variables evaluated at the earlier epoch, designated by the ordinal number n. All other symbols representing variables do so for the advanced epoch $n + 1$; for simplicity the superscript $n + 1$ is suppressed. It will be noted that the time derivatives are represented in terms of "backward" differences (i.e., $\Delta t = t^{n+1} - t^n$), and that therefore the time dependence is not symmetric. At the expense of some slight complexity it would be quite easy to average all quantities at the two epochs and thereby achieve a time-centered form. However, the presently adopted form is to be preferred over the centered one. It can be shown for the diffusion equation (cf. Richtmyer 1957) that the backward scheme causes short wavelength errors to damp out quickly, while the centered scheme allows them to die slowly in an overdamped oscillatory way. Since we use time steps sufficiently large that short wavelength effects do, in fact, physically damp out quickly, we prefer the non-symmetric scheme.

Not all the symbols displayed in our difference equations represent independent physical variables. The pressure, the internal energy, the opacity, and the energy generation rate are functions of temperature, density, and chemical composition. For present purposes we are not concerned with the precise expression for these functions but merely suppose that they are provided in some appropriate form. We regard the difference equations as conditions on the four variables r, F, T, and q.

The choice of the geometric mean for the effective value of ϵ, the rate of release of nuclear energy, is based on its tendency to vary rapidly from point to point. Actually there is no substitute for fine zoning in the presence of rapid variations of important variables, and there can be no justification of any scheme of averaging if variations are not restricted to reasonable levels.

The relevance of equation (25) or equation (26) depends on the usual considerations of stability against convection. The location of boundaries between convective and nonconvective regions is determined by the condition that a critical value of a stability criterion is just achieved on the convective side of the interface. The technical details

associated with the placing of these boundaries have presented troublesome problems whose resolution has been achieved only after considerable experimentation with various devices. One obvious scheme which was tried uses a mesh point for which ξ at the interface is a variable and is determined by the stability criterion used as an auxiliary condition. For reasons which are not entirely clear we did not succeed with this procedure because of an inherent tendency to create a numerical instability of an oscillatory character.

The procedure finally adopted is the following. When no convective region is present it is not necessary to determine the positions of the two boundaries, and the final model can be computed at once. When a single convective region exists (core or envelope), the boundary is set provisionally to coincide with each of two consecutive mesh points, in turn. For each case the model is computed and stored, and the stability criterion, whose vanishing determines the boundary,

$$S = \frac{dT}{dP} - \left(\frac{dT}{dP}\right)_{\text{ad}} \tag{27}$$

is evaluated on the convective side of the boundary. Clearly it is possible to find a pair of models having S values of opposite signs. Then the true boundary lies between the two provisional boundaries, and linear interpolation between the two computed models (using the S values to determine the weights) gives the final values of all quantities for the current time step. When both a convective core and a convective envelope are present, a minimum of three models will be needed for interpolation. How these may be found can be seen from Figure 1. The two axes are each representations of ξ, the abscissa for the core boundary, ξ_c, and the ordinate for the envelope boundary, ξ_e. The values of ξ at the mesh points are represented by a grid of horizontal and vertical lines. In the manner described above, we assume the core and envelope boundaries to coincide with some pair of mesh points (always requiring that $\xi_e > \xi_c$); in terms of Figure 1 this amounts to assuming that the point (ξ_c, ξ_e) coincides with some lattice point of the grid (e.g., point A). A model is computed and stored, and S is found to have the values $S_c^{(1)}$ and $S_e^{(1)}$ at the two boundaries. Depending on the signs of these, the representative point is then moved from that lattice point to one of its four *diagonal* neighbors; a second model is computed and stored separately from the first, and the values $S_c^{(2)}$ and $S_c^{(2)}$ are calculated. By letting the representative point move in such diagonal steps, it is possible eventually to locate the square $ABCD$ containing the true values of ξ_c and ξ_e. This will happen when two models are obtained giving opposite signs for $S_c^{(1)}$ and $S_c^{(2)}$ and for $S_e^{(1)}$ and $S_e^{(2)}$. Such a pair of provisional representative points might be either A and C or B and D in the drawing. If they are A and C, say, then one can examine the four S values to estimate whether B or D is likely to be better for computing the third model. When the three models have been calculated, the *six* S values are used to find interpolation weights, and the interpolated values of all stored quantities are determined and used as the final values for the current time step. In practice it is found that comparatively little searching is needed to bracket the core and/or envelope boundary by the above procedure.

The difference equations must be supplemented by appropriate boundary conditions. Two obvious (but essential) ones are

$$r_0 = 0 \tag{28}$$

and

$$l_0 = 0\,. \tag{29}$$

At the surface the boundary conditions are involved in the complexities of the stellar atmosphere. Here the physical description requires more parameters and, hence, additional and more complex equations. It is convenient to handle these matters with a sepa-

rate program which treats the outermost zone of the star from $j = J - 1$ to $j = J$. For our present purposes we shall suppose that this program determines the following quantities which are functions of the total radius R and the total luminosity L:

$$r_{J-1} = f_1(R, L), \tag{30}$$

$$F_{J-1} = f_2(R, L), \tag{31}$$

$$T_{J-1} = f_3(R, L), \tag{32}$$

and

$$q_{J-1} = f_4(R, L). \tag{33}$$

These quantities also involve the total mass and the surface values of the chemical composition, which are here treated as constants. In point of fact these functions are best determined by means of interpolation among a set of four suitably chosen discrete cases. The choice of points and scheme of interpolation are described in Section V. The basic

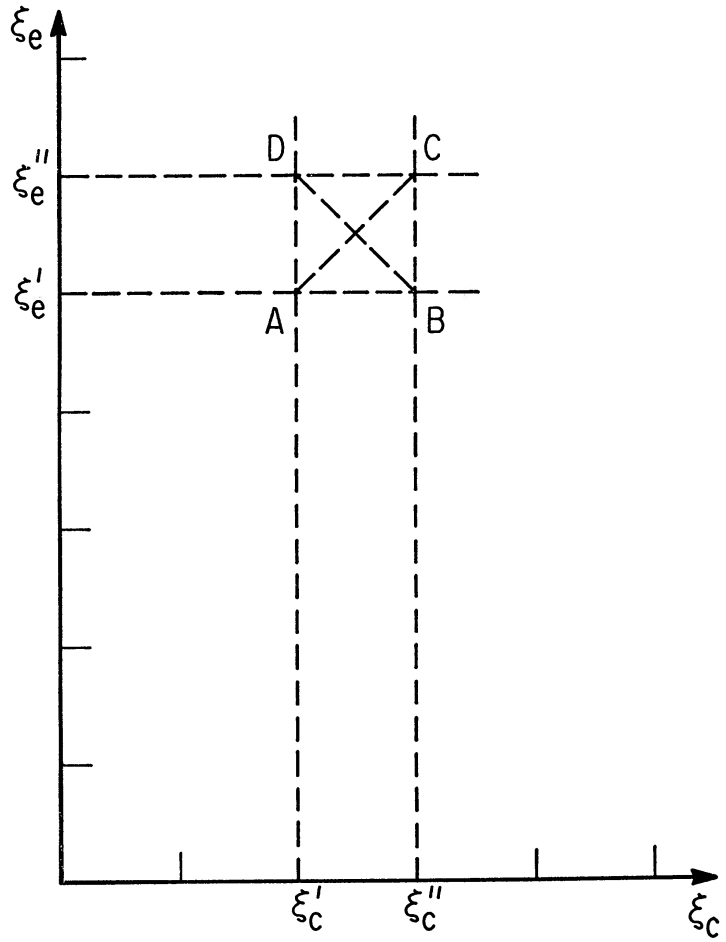

FIG. 1.—Here ξ_c is the Lagrangian coordinate of the outer boundary of the convective core, and ξ_e that of the inner boundary of the convective envelope. The symbols ξ_c', ξ_c'', and ξ_e', ξ_e'' designate provisional values for which, in certain combinations, complete stellar models are obtained. They fall on regular mesh points and are represented by the corners of one of the four triangles defined by the points A, B, C, and D. The triangle incloses the representative point for the configuration that satisfies the boundary conditions and which is obtained by interpolation among the three models.

integration needed to determine $f(R, L)$ will be the subject of a forthcoming report by M. S. Vardya. Where convection prevails in the outer layers the Böhm-Vitense (1958) model is used. The effects of sphericity are included, as well as those due to the dissociation of molecules.

An enumeration of the equations and of the unknowns reveals that we now have a complete system of equations: the difference equations (22)–(26), and the boundary conditions (28)–(33).

IV. SOLUTION OF THE DIFFERENCE EQUATIONS

In order to obtain a description of the solution of the difference equations in a concise form, we adopt a vector notation.

The first two difference equations (22) and (23) may be written in vector notation as

$$\phi_{j+1/2}\,(u_j, v_j; u_{j+1}, v_{j+1}) = 0\,, \tag{34}$$

while the third and fourth equations, (24) and (25) or (26), for radiative or convective equilibrium, respectively, are written

$$\psi_{j+1/2}\,(u_j, v_j; u_{j+1}, v_{j+1}) = 0\,. \tag{35}$$

Thus $\phi_{j+1/2}$ and $\psi_{j+1/2}$ are two-component vectors, each a function of the four vectors $u_j, v_j, u_{j+1}, v_{j+1}$, where

$$u_j = \begin{pmatrix} r_j \\ F_j \end{pmatrix} \quad \text{and} \quad v_j = \begin{pmatrix} T_j \\ q_j \end{pmatrix}.$$

The boundary conditions (28) and (29) at the center become

$$u_0 = 0\,. \tag{36}$$

The fitting of the outer zone leads to two equations derived from equations (30), (31) and (32), (33):

$$u_{J-1} - f(u_J) = 0 \tag{37}$$

and

$$v_{J-1} - g(u_J) = 0\,. \tag{38}$$

Let u_j, v_j be approximations to the correct solution for $\phi_{j+1/2}$, $\psi_{j+1/2}$ and let δu_j and δv_j be first-order corrections to them. These corrections will not all be zero unless $\phi_{j+1/2}$, $\psi_{j+1/2}$ and the left sides of equations (37) and (38) are zero. This will not, in general, happen. The variational forms of equations (34) and (35) then become

$$\begin{aligned} &\phi_{j+1/2} + \delta u_j \frac{\partial}{\partial u_j}\phi_{j+1/2} + \delta v_j \frac{\partial}{\partial v_j}\phi_{j+1/2} \\ &+ \delta u_{j+1} \frac{\partial}{\partial u_{j+1}}\phi_{j+1/2} + \delta v_{j+1} \frac{\partial}{\partial v_{j+1}}\phi_{j+1/2} = 0 \end{aligned} \tag{39}$$

and

$$\begin{aligned} &\psi_{j+1/2} + \delta u_j \frac{\partial}{\partial u_j}\psi_{j+1/2} + \delta v_j \frac{\partial}{\partial v_j}\psi_{j+1/2} \\ &+ \delta u_{j+1} \frac{\partial}{\partial u_{j+1}}\psi_{j+1/2} + \delta v_{j+1} \frac{\partial}{\partial v_{j+1}}\psi_{j+1/2} = 0\,. \end{aligned} \tag{40}$$

The tensors $(\partial/\partial u_j)\phi_{j+1/2}$, etc., are arrays of partial derivatives of the term in the difference equations (22)–(26) with respect to the variables r, F, T, and q for both subscripts j and $j + 1$.

Similarly the boundary condition at the center, equation (36), leads to the variational equation

$$\delta u_0 = 0 , \tag{41}$$

while at the outside equations (37) and (38) lead to

$$(u_{J-1} - f) + \delta u_{J-1} - \delta u_J \frac{\partial}{\partial u_J} f = 0 \tag{42}$$

and

$$(v_{J-1} - g) + \delta v_{J-1} - \delta u_J \frac{\partial}{\partial u_J} g = 0 . \tag{43}$$

The solution of the linearized equations must be organized carefully, since the grand matrix of the system is definitely ill-conditioned. This is apparent from the considerable change in order of magnitude of the quantities from center to surface. The solution must be based on some suitable scheme of elimination which uses linear equations derived from the original expressions. We now show that it is always possible to derive an equation which enables the elimination procedure to be organized in an especially efficient manner and which has the following form for all j:

$$\delta u_j + \delta v_j \alpha_j + \gamma_j = 0 . \tag{44}$$

In the case $j = 0$ we identify this expression with the boundary condition (41) and adopt $\alpha_0 = 0$ and $\gamma_0 = 0$. In order to show that this equation can be deduced for all values of j we proceed by mathematical induction. If it is valid for a particular j, we can, by direct substitution, eliminate δu_j from both equations (39) and (40), thereby obtaining two vector equations involving only δv_j, δu_{j+1}, and δv_{j+1}. From these two expressions we can now obtain one vector equation by eliminating δv_j. Moreover it is always possible to put the resultant equation in the form (44) with $j + 1$ replacing j, by formally solving for δu_{j+1}:

$$\delta u_{j+1} + \delta v_{j+1} \alpha_{j+1} + \gamma_{j+1} = 0 . \tag{45}$$

The coefficients in α_{j+1} and the components of γ_{j+1} are functions of α_j, γ_j, and of the various coefficients in equations (39) and (40). By methods analogous to Gaussian elimination we can construct from the equations involving δv_j, δu_{j+1}, and δv_{j+1} a vector equation which is independent of equation (45) and which has the form

$$\delta v_j \zeta_{j+1/2} + \delta u_{j+1} \eta_{j+1/2} + \delta v_{j+1} \beta_{j+1/2} + \theta_{j+1/2} = 0 , \tag{46}$$

where $\zeta_{j+1/2}$ is a triangular matrix with zeros below the principal diagonal. In fact it is always possible, but not essential, to obtain a form in which $\zeta_{j+1/2}$ is the unit matrix and $\eta_{j+1/2}$ is zero. However the more general form given by equation (46) is adequate and promotes economy in computing time. The tensors $\zeta_{j+1/2}$, $\eta_{j+1/2}$, and $\beta_{j+1/2}$ and the vector $\theta_{j+1/2}$ are also functions of α_j, of γ_j, and of the coefficients in equations (39) and (40).

The formal expressions determining the constants in equations (45) and (46) can now be used to generate them numerically for successive values of j from $j = 0$ to $j = J - 1$.

The final determination must now use the variational forms of the fitting conditions, equations (42) and (43). Using these two vector equations together with equation (44), as established for $j = J - 1$, we now obtain explicit numerical values for δu_{J-1}, δv_{J-1}, and δu_J. Then by means of equation (46) we evaluate the components δv_{J-2}. This in turn permits the evaluation of δu_{J-2} from equation (44). By successively applying equations (46) and (44) with decreasing values of j we obtain all values of the components of δu_j and δv_j.

The final step is the calculation of $u_j + \delta u_j$ and $v_j + \delta v_j$, which now replace the previous values of u_j and v_j.

The fractional corrections $\delta u_j/u_j$ and $\delta v_j/v_j$ are now examined to determine whether another iteration is required. If, for all values of j, they are within a properly chosen tolerance, the model is considered to be converged. Otherwise the entire process is repeated.

The over-all organization of the calculation is indicated in Figure 2. Each iteration for differential corrections is followed by a recalculation of the chemical composition as affected by thermonuclear reactions and mixing. In fact, these calculations are the first and last things done for a model.

Initial values for a particular epoch are determined by extrapolation from the previous two epochs. By doing this it is possible to cut down the total number of iterations needed.

V. MISCELLANEOUS CONSIDERATIONS

The preparation of a successful program for the automatic computation of stellar evolution must include provisions for various and numerous details of operation and organization. We consider some of these in this section.

In order to begin the calculation of the evolutionary track of a star this program must be provided with the total mass of the star, a beginning radius, and a chemical composition. Also required are the mass distribution, defined by $m(\xi)$ (which does not change with time) and an initial configuration giving first approximations for the variables r_j, F_j, T_j, q_j for each j. A procedure presently in use for generating these quantities is to begin with a set of values from a previous calculation and scale them homologously to meet the required total mass and initial radius as well as the required composition.

While the mass at the boundary and at the middle of each permanent zone is fixed by the generating program, it is necessary to provide for its calculation for the temporary mesh points. For this purpose the generating program calculates a sixth-order difference table which is kept as a permanent part of the calculations. Each time it is necessary to obtain the mass at a new value of ξ (as a result of insertion and deletion of temporary mesh points) it is interpolated by means of this difference table.

The consideration of a moving interface between radiative and convective regions presents certain special situations which need to be recognized and properly treated. Some of these are briefly mentioned here.

At the boundary of a convective region in the case of discontinuity in chemical composition the pressure and temperature are continuous, but the density is not. In order properly to represent this effect an additional mesh point is inserted at the core boundary on the radiative side such that $\xi_{j_c+1} = \xi_{j_c}$. Values at these two contiguous mesh points differ only when there is a discontinuity in chemical composition. In that case r_j, p_j, and T_j are identical for j_c and $j_c + 1$, but q_j, E_j, and the concentrations of the various chemical species may be different on the two sides of the interface. No temporary mesh points may be inserted between j_c and $j_c + 1$. The equation expressing the equality of the pressure at j_c and $j_c + 1$ serves to connect the two sides of the interface and permits a zonelike formalism which uses the regular coding to develop the possible discontinuities.

An additional artificial mesh point is inserted at the core boundary for the previous epoch (ξ_c^n). Then if, for instance, the core has been expanding and then begins to contract, it must cross, inward bound, this special mesh point and thus determine in an unambiguous way the switch from expanding core physics (chemical composition discontinuity at the interface) to contracting core physics (no discontinuity). Also the sweeping up of the peripheral composition by an expanding boundary can be described conveniently using the point at ξ_c^n.

In order to establish the correct timewise differences of q and E in equation (24) for a moving interface, it must be remembered that they represent the time derivatives for constant ξ. Values of q^n and E^n corresponding to the current position of ξ_c and ξ_e must replace those calculated for the moving interfaces at the previous epoch.

The representation of the pressure, the internal energy, and the opacity as functions of

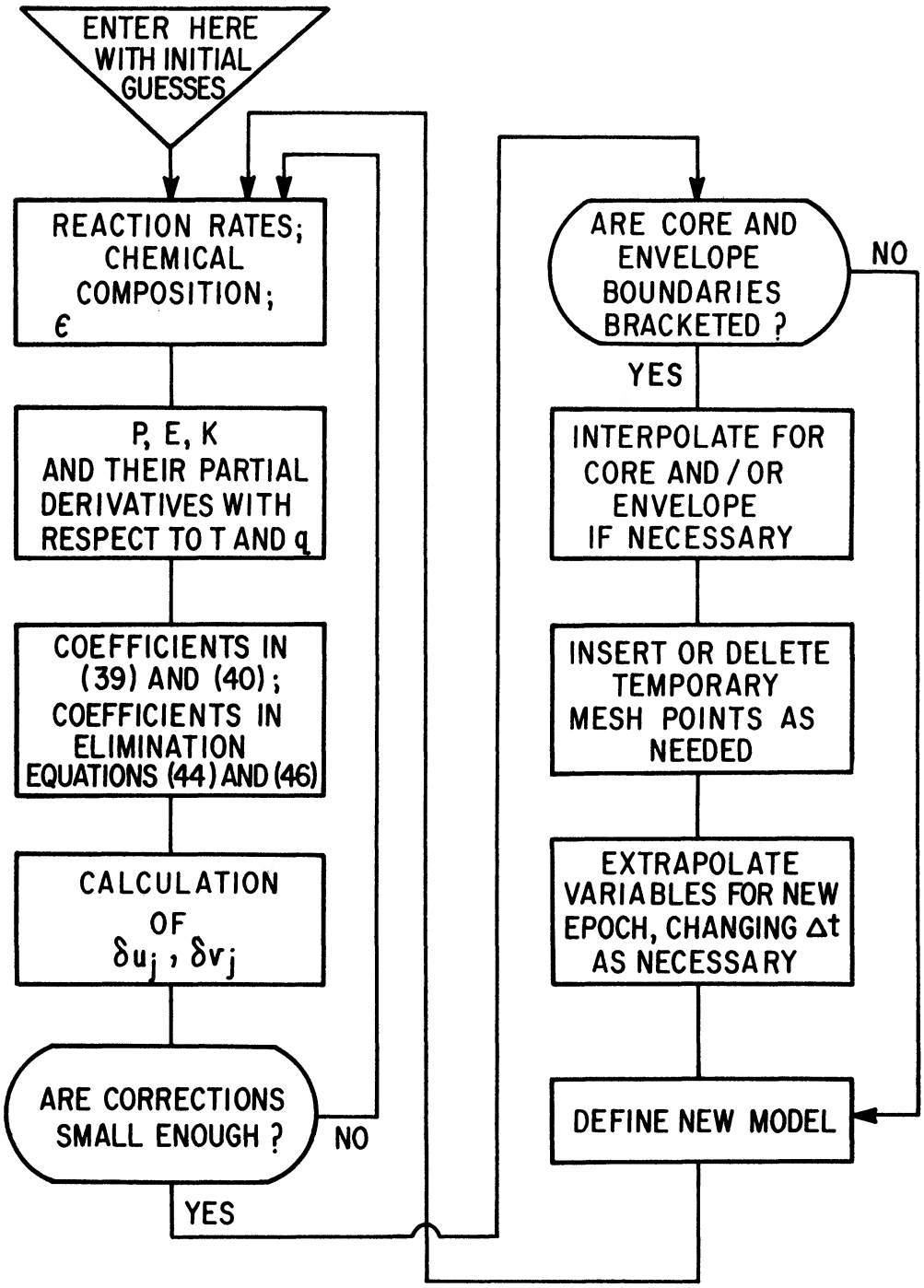

FIG. 2.—Block diagram giving the logical pattern for the ordering of calculations defining a configuration in an evolutionary sequence of models

density and temperature must be done in such a way as to assure their continuity. For example, allowance for degeneracy in the equation of state may be provided only when the effect is larger than certain tolerance limits, thus producing a slight discontinuity. This, in turn, leads to a discontinuity in the equations of condition. Sooner or later the computer will attempt to find a value of the pressure which just falls in the range of this discontinuity and will be unable to converge to definite values. The reason for this may be understood from a consideration of Figure 3. The function $f(x)$ has a discontinuity which encompasses the root x_0. By graphically following the Newton-Raphson technique one can readily verify that it will be completely incapable of converging to the root. The difficulty can be avoided by assuring complete continuity or by reducing the discontinuity to a level such that the criterion for convergence will tolerate the indeterminacy which is present.

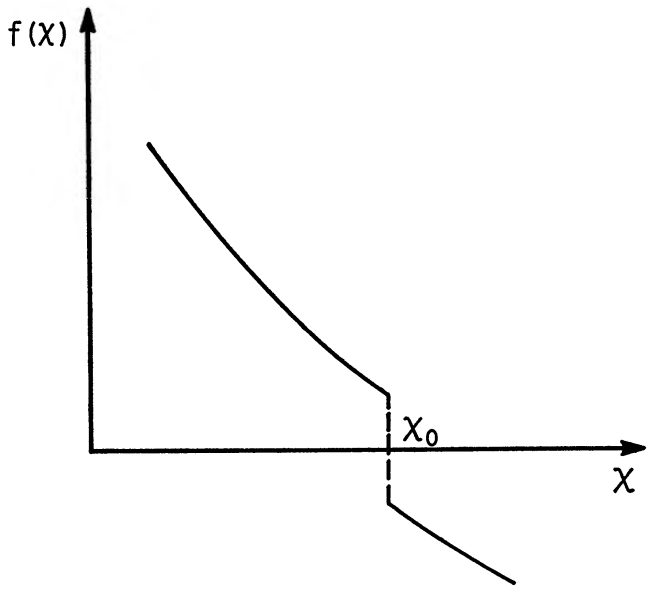

FIG. 3.—A function $f(x)$ has a discontinuity at x_0 which encompasses a root. The Newton-Raphson method (method of tangents) fails to converge unless the discontinuity is less than the tolerance adopted

In the multidimensional space of all of the increments δr_j, δF_j, δT_j, δq_j for all j in the Newton-Raphson iterative cycle there exists a limited region of convergence. Experience definitely indicates that the size of this region can be significantly increased by limiting the maximum increments of the variables. In locating the largest fractional change, $\delta r_j/r_j$, $\delta T_j/T_j$, $\delta q_j/q_j$, $\delta p_j/p_j$ are examined for all j, but $\delta F_j/F_j$ is examined only for $j = J$ (because F_j can temporarily become zero at some points within the star). If any of the fractional changes examined are greater than the prescribed limit all of the increments are reduced by a factor which will bring the largest fractional change within this limit.

As was mentioned in Section III the exterior boundary conditions are actually interpolated among four discrete cases. In the diagram (Fig. 4) representing the LR-plane, we use a grid such that each corner of a rectangle represents an actual atmosphere calculation giving r, F, T, q at $J - 1$ as functions of R and L. At any given time the star will be represented by a point within one of these rectangles, and the variational equations (42) and (43) are based on interpolation among the four corners. As the representative point for the star moves in this plane its coordinates are examined at each new iteration and if they do not place it more than 1 per cent outside its present rectangle, that rectangle is

considered adequate. The error in interpolation here is not great, and this device insures that the point will not erroneously move into a new square as a result of inaccuracies in the extrapolation to a new epoch. If the point has truly moved to a new rectangle in the grid the appropriate new R and/or L are determined and new sets of values are computed for the new corners. In moving to a new rectangle R and/or L are increased or decreased by a factor of 1.15.

The calculations relating to changes in composition involve substantial problems in numberical analysis. Since the reactions to be considered in a calculation are specific to the particular problem under investigation, we here omit detailed description of them and postpone their discussion to future reports on applications of this program. We have

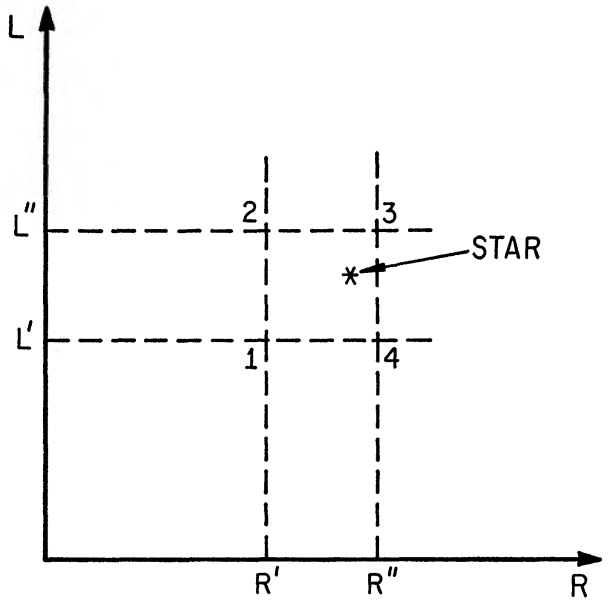

FIG 4.—Points *1*, *2*, *3*, *4* represent atmosphere calculations for configurations defined by L and R, in addition to fixed values of M and the composition. They provide boundary conditions to the interior integration by interpolation for the actual position of the representative point for the star in the L, R plane

found it convenient to program separately some of the individual reactions in the proton-proton chain and the CNO bi-cycle. In doing so, the adopted difference equations were designed to work for values of Δt which are either substantially larger or smaller than the mean life of the nuclear species to which a particular equation refers.

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